# CONVEX ENVELOPES OF MULTILINEAR FUNCTIONS OVER A UNIT HYPERCUBE AND OVER SPECIAL DISCRETE SETS

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Dedicated to Hoang Tuy on the occasion of his seventieth birthday

Abstract. In this paper, we present some general as well as explicit characterizations of the convex envelope of multilinear functions defined over a unit hypercube. A new approach is used to derive this characterization via a related convex hull representation obtained by applying the Reformulation-Linearization Technique (RLT) of Sherali and Adams (1990, 1994). For the special cases of multilinear functions having coefficients that are either all  $+1$  or all  $-1$ , we develop explicit formulae for the corresponding convex envelopes. Extensions of these results are given for the case when the multilinear function is defined over discrete sets, including explicit formulae for the foregoing special cases when this discrete set is represented by generalized upper bounding (GUB) constraints in binary variables. For more general cases of multilinear functions, we also discuss how this construct can be used to generate suitable relaxations for solving nonconvex optimization problems that include such structures.

## 1. INTRODUCTION

The construction of convex envelopes for nonconvex functions over convex sets plays an important role in solving both discrete and continuous nonconvex programming problems (see Horst and Tuy, 1993). Explicit closed-form formulae have been derived for many special cases such as for bivariate bilinear functions over rectangles (Al-Khayyal and Falk, 1983) and over D-polytopes (Sherali and Alameddine, 1990), for monomials defined over a unit hypercube (Crama, 1993, Glover and Woolsey, 1974, and Hansen and Simeone, 1990), for special quadratic multilinear functions defined over a unit hypercube (Rikun, 1996), for concave functions over

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polytopes or simplices (Pardalos and Rosen, 1987), and for certain classes of fixed-charge functions defined over hypercubes and special bounded knapsack constrained regions (Benson and Erenguc, 1988, and Denizel, Erenguc, and Sherali, 1995). These explicit formulae provide a set of tools that can be applied to more general problems that include such cases as substructures in order to generate useful relaxations. General convex envelope characterizations and results are also given in Falk (1969), Rockafellar (1970). McCormick (1976), Grotzinger (1985), Pardalos and Rosen (1987), and Horst and Tuy (1993) that can be used to derive tight convex underestimating functions for deriving relaxations and lower bounds within the context of branch-and-bound algorithms. In some cases, a combination of such explicit and relaxed convex envelope representations have been proposed. For example, Kalantari and Rosen (1986) show that given an indefinite quadratic function defined over a polytope, another special polytope can be generated that contains the given polytope such that over this regions, an explicit convex envelope of the given function can be constructed.

In this paper, we focus on multilinear functions  $\phi : H \subseteq R^n \to R$ , where

(1) 
$$
\phi(x) = \sum_{t \in T} \alpha_t \prod_{j \in J_t} x_j,
$$

and where  $H$  is a unit hypercube given by

(2) 
$$
H = \{x : 0 \le x \le e\},\
$$

where  $e$  is a vector of *n*-ones. Here, the set  $T$  indexes the terms that define  $\phi$ , and for each term  $t \in T$ ,  $\alpha_t$  is a real coefficient and  $J_t \subseteq N = \{1, \ldots, n\}$ is an associated nonempty set of distinct variable indices represented in the corresponding product term. This is known as a multilinear function since  $\phi$  is linear in each variable  $x_j$  when the other variables in N are fixed at some values. In particular, when  $\phi$  contains all possible distinct products of the variables  $x_1, \ldots, x_n$  taken m at a time, where  $2 \le m \le n$ , and each such term has a unit coefficient, we will refer to such a multilinear function as a *combinatorial multilinear function*  $(CMF)$  of order m, and denote it by  $\phi^m$ . Mathematically, this function is given by

(3) 
$$
\phi^m(x) = \sum_{\substack{J \subseteq N \\ |J| = m}} \Big[ \prod_{j \in J} x_j \Big].
$$

Note that such CMF functions represent the sum of  $m$ -way combinations of variables, and might arise in combinatorial constraints involving binary variables or as subsets of multilinear objective or constraint functions in nonlinear 0-1 programs (see Balas and Mazzola, 1984a, b, Hansen, 1979, and Hansen, Jaumard, and Mathon, 1989). Recently, Rikun (1996) has developed an explicit formula for the (polyhedral) convex envelope of  $\phi^m$ given by (3) over H, for the special case of  $m = 2$ , and has shown that this yields a significantly tighter representation than that obtained via standard linearization approaches for nonlinear 0-1 problems. Rikun states this formula and *verifies* that it represents the convex envelope of  $\phi^2(x)$ over  $H$  by applying a set of general results that specify certain sufficient conditions for a given function to be the convex envelope of a continuously differentiable function defined over a polytope, given that this envelope is polyhedral. In contrast, using a new approach based on characterizing the convex hull for certain discrete sets via the Reformulation-Linearization Technique (RLT) of Sherali and Adams (1990, 1994) we show how this formula can be constructively derived. Moreover, we derive explicit formulae for both the convex and concave envelopes of  $\phi^m$  of general order  $m \leq n$ , defined over the unit hypercube H. We also characterize the convex envelope of  $\phi$  when its definition is restricted to a set of discrete binary solutions. In particular, this leads to similar closed-form formulae for the case when this discrete set is defined by generalized upper bounding (GUB) constraints in binary variables, given by

(4) 
$$
H_{GUB} = \left\{ x : \sum_{j \in S_r} x_j \le 1 \text{ for } r = 1, \dots, R, x \text{ binary} \right\},\
$$

where  $\bigcup^R$  $i=1$  $S_i = N$ , and  $S_i \cap S_j = \emptyset \ \forall i \neq j$ . Such GUB constraints arise frequently in applications involving multiple choice constraints, and represent an important structure in 0-1 optimization for which tight polyhegral representation can be quite usefull (see Nemhauser and Wolsey, 1988, Wolsey, 1990, and Sherali and Lee, 1995). For the more general case of  $\phi$  given by (1), we discuss how our approach can be used to generate suitable underestimating representations for constructing convex or polyhedral relaxations for nonconvex problems that subsume such structures.

The remainder of this paper is organized as follows. We begin by presenting some preliminary definitions and results in Section 2, and develop a general characterization of the convex envelope of multilinear functions over a unit hypercube, as well as over special discrete sets by applying the RLT procedure. Using this characterization, we then derive explicit

formulae for the convex envelope of  $\phi^m(x)$  over H in Section 3, and for concave envelope of  $\phi^m(x)$  over H in Section 4, for any  $m \leq n$ . These formulae are extended to the case of GUB constrained regions  $H_{GUB}$ given by (4) in Section 5. Finally, in Section 6, we discuss the generation of relaxations for more general cases using the construct of Section 2.

## 2. Preliminary results and some general convex envelope characterizations

In this section, we present a general approach for constructing convex envelopes, and show how the Reformulation-Linearization Technique (RLT) of Sherali and Adams (1990, 1994) can be used to characterize, in particular, the convex envelope of  $\phi$  given by (1) over a unit hypercube H.

To begin with, consider the following definition.

**Definition 1** [Horst and Tuy, 1993]. The *convex envelope* of a function  $\phi$ taken over a nonempty convex subset S of its domain is that function  $\phi_S$ for which:

(a)  $\phi_S$  is a convex function defined over S,

(b)  $\phi_S(x) \leq \phi(x)$  for all  $x \in S$ , and

(c) if  $\phi' : S \to R$  is a convex function that satisfies  $\phi'(x) \leq \phi(x)$  $\forall x \in S$ , then

 $\phi'(x) \leq \phi_S(x) \quad \forall x \in S.$ 

Equivalently, the convex envelope of  $\phi$  over the convex set S is given by the pointwise supremum of all convex, or even simply affine, underestimating functions for  $\phi$  over the set S.

There exists a direct relationship between convex envelopes and convex hulls that provides a useful facility for constructing the convex envelope of a nonconvex function  $\phi$  over a given convex set S. Consider a lower semicontinuous function  $\phi : S \to R$ , where  $S \subseteq R^n$  is a nonempty, compact, convex set. Recall that (see Bazaraa et al., 1993 for related definitions) the epigraph of  $\phi$  over the set S, denoted  $E_S(\phi)$ . is defined by

(5) 
$$
E_S(\phi) = \{(x, z) : x \in S, z \ge \phi(x)\}.
$$

Let us denote the *convex hull* of this set by *conv*  $E_s(\phi)$ . Then, we have the following result.

**Theorem 1.** Let  $\phi : S \to R$  be a lower semicontinuous function, where  $S \subseteq R^n$  is convex and compact, and let  $E_S(\phi)$  be as defined by (5). Then

(6) conv 
$$
E_s(\phi) = \{(x, z) : x \in S, z \ge \phi'(x)\} \Leftrightarrow \phi'(x) = \phi_S(x) \quad \forall x \in S.
$$

Proof. The proof follows by Horst and Tuy (1993, Lemma IV.1), and Sherali and Alameddine (1992, Theorem 4), by noting that conv  $E_S(\phi)$  is a closed set since  $\phi$  is lower semicontinuous and S is a convex, compact set.  $\Box$ 

Observe that Theorem 1 is quite intuitive in that the convex hull of  $E_S(\phi)$  is the smallest convex set that contains  $E_S(\phi)$ , and the convex envelope  $\phi_S(x)$  of  $\phi$  over the set S is, by definition, the tightest convex underestimating function for  $\phi$  over the set S. Note that if the set S in Theorem 1 is nonempty, closed and convex, but not necessarily bounded, then the convex hull operator in (6) should be replaced by the closure of the convex hull for this result to hold true.

The construct embodied by Theorem 1 provides a useful technique for computing the convex envelope of a given function  $\phi$  over a convex set S. In particular, if the epigraph  $E_S(\phi)$  defined in (5) can be represented using binary variables, for example, in a manner that facilitates the construction of its convex hull, then Theorem 1 can be gainfully employed to derive the convex envelope of  $\phi$ . Denizel, Erenguc, and Sherali (1995) analyze certain instances of fixed-charge functions for which this approach turns out to be particularly convenient. As we shall presently see, when this concept is used in concert with the RLT approach, we can derive a usefull tool for analyzing our problem at hand. This is characterized by the following result.

**Theorem 2.** Let  $\phi: H \to R$  be a multilinear function given by (1), where H is a unit hypercube as defined in (2). Then, the convex envelope of  $\phi$ over the set H is given by

(7a) 
$$
\phi_H(x) = \max \Big\{ \sum_{j \in N} \pi_j^k x_j - \pi_0^k, \ k = 1, ..., K \Big\},\
$$

where  $(\pi^k, \pi_0^k)$ ,  $k = 1, ..., K$  represent the set of vertices of the set  $\Pi$ , denoted vert  $(\Pi)$ , where  $\Pi$  is given by

(7b) 
$$
\Pi = \Big\{ (\pi, \pi_0) : \sum_{j \in J} \pi_j - \pi_0 \leq \beta_J \quad \forall J \subseteq N \Big\},\
$$

and where, letting  $x(J)$  denote the solution

(7c)  $x(J) = (x_j = 1, \quad \forall j \in J, \ x_j = 0, \quad \forall j \in \overline{J} \equiv N - J), \quad \forall J \subseteq N,$ we have

(7d) 
$$
\beta_J \equiv \phi(x(J)), \quad \forall J \subseteq N.
$$

*Proof.* Let the epigraph of  $\phi$  over  $S \equiv H$  be given by (5). Then we have

(8) 
$$
\operatorname{conv} E_H(\phi) = \operatorname{conv} \{(x, z) : z \ge \phi(x), x \text{ binary}\}.
$$

This follows since for any affine function  $\psi x + \psi_0$ , we have  $\phi(x) \ge \psi x + \psi_0$ This follows since for any affine function  $\psi x + \psi_0$ , we have  $\phi(x) \geq \psi x + \psi_0$ <br>  $\forall x \in H \Leftrightarrow \min \{\phi(x) - \psi x - \psi_0 : x \in H\} \geq 0 \Leftrightarrow \min \{\phi(x) - \psi x - \psi_0 : x \in H\}$  $\forall x \in H \Leftrightarrow \min{\{\psi(x) - \psi x - \psi_0 : x \in H\}} \geq 0 \Leftrightarrow \phi(x) \geq \psi x + \psi_0 \,\,\forall x \text{ binary}.$  Here, we have used the fact that the minimum of  $\phi(x) - \psi x - \psi_0$  over  $x \in H$  is attained at a binary solution since  $\phi$  is multilinear and H represents a set of separable constraints  $0 \leq x_j \leq 1$ , for  $j = 1, \ldots, n$ . Hence, the set of affine underestimating functions for  $\phi$  over H coincide with the set of affine functions that underestimate  $\phi$  over binary values of x.

Now, using the RLT approach of Sherali and Adams (1990, 1994), the convex hull on the right-hand side of (8) can be written as follows.

(9)  
\n
$$
\operatorname{conv}\{(x, z) : z \ge \phi(x), x \text{ binary}\} =
$$
\n
$$
\{(x, z) : x_j = \sum_{\substack{J \subseteq N \\ j \in J}} y_J \quad \forall j \in N,
$$
\n
$$
z = \sum_{J \subseteq N} \theta_J, \ \theta_J \ge \beta_J y_J, \quad \forall J \subseteq N,
$$
\n
$$
\sum_{J \subseteq N} y_J = 1, \text{ and } y_J \ge 0, \ \forall J \subseteq N\},
$$

where  $\theta_J$  and  $y_J, J \subseteq N$ , are suitable linearization variables that define the convex hull as in (9) in a higher dimensional space following Sherali and Adams, and where  $\beta_J$  is given by (7d)  $\forall J \subseteq N$ . Hence, using (8) and (9) along with linear programming duality, and noting that  $\beta_{\emptyset} \equiv 0$ , and that  $y_{\emptyset}$  is a slack variable in the convexity constraint in (9), we have

$$
\text{conv } E_H(\phi) = \left\{ (x, z) : \text{ there exist } y_J, J \subseteq N, J \neq \emptyset \text{ such that } \right\}
$$

$$
z \ge \sum_{J \neq \emptyset} \beta_J y_J, \text{ and where } \sum_{J:j \in J} y_J = x_j \quad \forall j \in N,
$$

$$
\sum_{J \neq \emptyset} y_J \le 1, y_J \ge 0 \quad \forall J \neq \emptyset \right\}
$$

$$
= \left\{ (x, z) : 0 \le x \le e \text{ and } z \ge \text{minimum} \{ \sum_{J \neq \emptyset} \beta_J y_J : \sum_{J \neq \emptyset} y_J = x_j \ \forall j \in N, \sum_{J \neq \emptyset} y_J \le 1, \text{ and } y_J \ge 0 \ \forall J \neq \emptyset \} \right\}
$$

$$
= \left\{ (x, z) : 0 \le x \le e, \text{ and } z \ge \text{maximum} \{ \sum_{j \in N} \pi_j x_j - \pi_0 \}
$$

$$
\text{subject to } \sum_{j \in J} \pi_j - \pi_0 \le \beta_J \ \forall J \neq \emptyset, \ \pi_0 \ge 0 \right\}
$$

$$
= \left\{ (x, z) : 0 \le x \le e, \right.
$$

$$
(10)
$$
and  $z \ge \text{maximum} \{ \sum_{j \in J} \pi_j^k x_j - \phi_0^k, \ k = 1, ..., K \} \right\},$ 

where  $(\pi^k, \pi_0^k)$ ,  $k = 1, ..., K$ , represent the vertices of  $\Pi$  given by (7b). (Note that for  $J = \emptyset$  in (7b), we have  $\beta_J \equiv 0$ , so that the corresponding constraint reads as  $\pi_0 \geq 0$ . By Theorem 1 and Equation (10), we have (7a) holding true, and this completes the proof.  $\Box$ 

j∈N

Corollary 1. Let S be a polytope contained in the unit hypercube H that has binary vertices, and let  $\phi$  be given by (1). Then

$$
\text{conv }\big\{(x,z) : x \in S, \ x \ binary, \ z \ge \phi(x)\big\}
$$
\n
$$
\text{(11a)} = \Big\{(x,z) : x \in S, \ z \ge \sum_{j \in N} \pi_j^k x_j - \pi_0^k \quad \forall (\pi^k, \pi_0^k) \in \text{vert }\Pi(S)\Big\},\
$$

where

(11b) 
$$
\Pi(S) = \left\{ (\pi, \pi_0) : \sum_{j \in J} \pi_j - \pi_0 \le \beta_J \ \forall J \in F \right\},\
$$

and where

 $(11c)$   $F =$  $\overline{a}$  $J \subseteq N : x(J)$  is feasible to (is a vertex of)S ª ,

and  $x(J)$  and  $\beta_J$  are given by (7c) for each  $J \in F$ .

*Proof.* From Sherali and Adams (1990, 1994), conv  $\{(x, z) : x \in S, x \text{ binary},$  $z \geq \phi(x)$  is given by (9) with the added restriction that  $y_J \equiv 0$  if  $J \notin F$ . Hence, following the derivation of (10) with this added restriction, we obtain the characterization specified by (11), and this completes the proof.  $\Box$ 

Note that Corollary 1 asserts that if we are given a multilinear function  $\phi$  defined over a polytope S that has binary vertices, as for example if S is defined by totally unimodular constraints in variables bounded by  $H$ , and if we are interested in constructing a tight convex underestimator of  $\phi$ only over the set of vertices of S, then we can define  $\phi_b$  to be the function such that

(12a) 
$$
\phi_b(x) = \begin{cases} \phi_b(x) & \text{if } x \text{ is binary,} \\ \infty & \text{otherwise,} \end{cases}
$$

and then accordingly construct the convex envelope  $\phi_{bS}(x)$  of  $\phi_b$  over the set S. By Theorem 1 and Corollary 1, we would then obtain

(12b) 
$$
\phi_{bS}(x) = \max\Big\{\sum_{j\in N}\pi_j^k x_j - \pi_0^k : (\pi^k, \pi_0^k) \in \text{vert }\Pi(S)\Big\},\,
$$

where  $\Pi(S)$  is defined by (11b, c). The polyhedral function (12b) would hence provide a valid underestimator for  $\phi$  over binary solutions in S, and could therefore be used to construct suitable continuous relaxations for discrete problems that contain such a structure. Later in Section 5, we will apply this result to the important special case where  $S$  is defined by GUB constraints as in the continuous relaxation of (4).

## 3. Convex envelope of combinatorial multilinear functions over a unit hypercube

In this section, we will show that the convex envelope of the function  $\phi^m(x)$  defined in (3) for any  $m \leq n$  over a unit hypercube H is given by

(13) 
$$
\phi_H^m(x) = \text{maximum} \Big\{ 0, \Big( \frac{k}{m-1} \Big) \sum_{j=1}^n x_j - (m-1) \Big( \frac{k+1}{m} \Big),
$$

$$
\text{for } k = m-1, \dots, n-1 \Big\}.
$$

We *derive* this result (as opposed to *verifying* this claim) by applying Theorem 2, and characterizing the set of vertices of the set Π defined by

(7b). Note that for  $\phi^m$  given by (3), we have from (7c) and (7d) that

(14) 
$$
\beta_J = \begin{cases} 0 & \text{if } |J| = k, \text{ for } k = 0, 1, ..., m - 1, \\ {k \choose m} & \text{if } |J| = k, \text{ for } k = m, ..., n, \end{cases}
$$

for each  $J \subseteq N$ . Substituting this in (7b), we obtain

$$
\Pi = \Big\{ (\pi, \pi_0) :
$$

(15a) 
$$
\sum_{j\in J}\pi_j - \pi_0 \leq 0 \quad \forall J \subseteq N \ni |J| = k, \text{ for } k = 0, 1, \dots, m-1,
$$

(15b) 
$$
\sum_{j\in J} \pi_j - \pi_0 \le {k \choose m} \quad \forall J \subseteq N \ni |J| = k, \text{ for } k = m, \dots, n.
$$

The following result characterizes the vertices of (15), and hence establishes  $(13)$ .

**Theorem 3.** The extreme points of the set  $\Pi$  defined in (15) are given by  $(\pi = 0, \pi_0 = 0)$  and

(16) 
$$
\left(\pi_j = \left(\frac{k}{m-1}\right) \forall j \in N, \ \pi_0 = (m-1)\left(\frac{k+1}{m}\right)\right),
$$

for  $k = m - 1, \ldots, n - 1$ , and so,  $\phi_H^m(x)$  is given by (13).

*Proof.* Since  $\Pi \subset R^{n+1}$ , its vertices are feasible solutions at which some  $(n+1)$  linearly independent defining hyperplanes are binding. If (15a) for  $k = 0$  is binding, i.e.,  $\pi_0 = 0$ , then (15a) for  $k = 1$  asserts that  $\pi_i \leq 0$  $\forall j \in N$ , and these restrictions then imply the other defining constraints in (15). Hence, if  $\pi_0 = 0$  at a vertex of  $\Pi$ , we must have  $\pi_j = 0 \ \forall j \in N$ , and this produces the vertex  $(\pi = 0, \pi_0 = 0)$  of  $\Pi$ .

Next, consider any  $1 \leq k' < m-1$ , and suppose that for some  $J = J_p$ with  $|J_p| = k'$ , a constraint from (15a) is binding at a vertex of  $\Pi$ , so that

(17a) 
$$
\sum_{j \in J_p} \pi_j - \pi_0 = 0.
$$

Note that the constraints in (15a) that correspond to  $J = J_p \cup j$  for  $j \notin J_p$  (where  $k = k' + 1$ ) together with (17a), imply that

(17b) 
$$
\pi_j \leq 0 \quad \forall j \notin J_p.
$$

Moreover, for any  $k = (k'+2), \ldots, n$ , we get using (17) and the constraints in (15a) for  $k = 0, \ldots, k'$  that

$$
\sum_{j\in J}\pi_j-\pi_0\leq \sum_{j\in J\cap J_p}\pi_j-\pi_0\leq 0.
$$

Hence, all the constraints for  $k \geq k' + 2$  in (15) are then implied, and therefore do not figure into determining a vertex of Π in this case. But all the constraints in (15a) are binding at the above extreme point ( $\pi =$ 0,  $\pi_0 = 0$ , and so, this is the only vertex at which any constraint of type (17a) is binding.

Proceeding inductively, now suppose that for some  $k' \in \{m-1,\ldots,n-1\}$ 1}, we have that at some vertex of  $\Pi$ , all the constraints in (15) for  $k < k'$ are inactive, while some constraint corresponding to  $J = J_p$  with  $|J_p| = k'$ is active or binding. Hence, we have

(18a) 
$$
\sum_{j\in J_p} \pi_j - \pi_0 = \binom{k'}{m},
$$

where we assume that  $\binom{k'}{k}$ m ´  $\equiv 0$  whenever  $k' < m$ . From the constraints in (15) corresponding to  $J = J_p \cup j$  for  $j \notin J_p$ , so that  $|J| = k' + 1$ , we get using (18a) that

(18b) 
$$
\pi_j \leq {k'+1 \choose m} - {k' \choose m} = {k' \choose m-1} \ \forall j \notin J_p.
$$

Now, consider the constraints in (15) for  $k = k' + r$ , where  $r \ge 1$ . Note that so long as (15) is satisfied for  $k \leq k'$  and that (18) holds true, we get

(19) 
$$
\sum_{j\in J} \pi_j - \pi_0 = \Big[ \sum_{j\in J\cap J_p} \pi_j - \pi_0 \Big] + \sum_{j\in J-J_p} \pi_j \le \binom{k'}{m} + r \binom{k'}{m-1} \le \binom{k'+r}{m}.
$$

The first inequality in (19) holds true since by (15b), we have

$$
\sum_{j \in J \cap J_p} \pi_j - \pi_0 \le {\lceil J \cap J_p \rceil \choose m} \le {\binom{k'}{m}}
$$

and since (18b) is satisfied  $\forall j \notin J_p$ , and the second inequality in (19) holds true since the number of ways  $m$  items can be selected from some

 $k'$  plus r items exceeds the number of ways m items can be selected from the k' items, plus the number of ways  $(m-1)$  items can be selected from the  $k'$  items along with just one of the r items taken in turn. (Note that this inequality also holds true for  $k' = m - 1$  and  $r \ge 1$ ). Therefore, we have shown that under this case, if (18a) holds true, then (18b) must be satisfied, and that all the other inequalities in (15) for  $k \geq k' + 1$  would then automatically be satisfied and so would not figure into determining the corresponding vertex. Consequently, the possible defining hyperplanes that could determine a vertex corresponding to this case must come from the following constraints:

(20) 
$$
\begin{cases} \text{constraints in (15) for } k = k' \\ \text{including the one for } J = J_p \end{cases} \cup \{\text{constraints in (18b)}\}.
$$

Consider now the situation in which all the constraints from the first set within  $\{\cdot\}$  in (20) are binding. By symmetry, this gives via (15) that

(21) 
$$
\pi_j \equiv \pi \quad \forall j \in N, \text{ where } k'\pi - \pi_0 = \binom{k'}{m}.
$$

Hence, in order to obtain  $(n + 1)$  linearly independent hyperplanes, we must have some from (18b) also binding, where any of these uniquely gives along with (21) that

(22) 
$$
\pi_j = \pi = \binom{k'}{m-1} \forall j \in N, \text{ and}
$$

$$
\pi_0 = k' \binom{k'}{m-1} - \binom{k'}{m} = (m-1) \binom{k'+1}{m}.
$$

Hence,  $(22)$  defines a vertex of  $\Pi$ , and moreover, since all the constraints in (20) are active at the solution (22), no subset of these could yield a set of  $(n + 1)$  linearly independent hyperplanes that produce a different vertex of Π. Therefore, (22) is the only vertex obtained for this case, for each  $k' = m - 1, \ldots, n - 1$ . This establishes (16). Hence, by Theorem 2, (13) holds true and this completes the proof.  $\Box$ 

**Example 1** (Rikun's (1986) result as a special case). Note that for  $m = 2$ , we have  $\overline{\phantom{a}}$ 

$$
\phi^2(x) \equiv \sum_{i < j} x_i x_j
$$

and by (13), we obtain

$$
\phi_H^2(x) = \text{maximum } \Big\{ 0, k \sum_{j=1}^n x_j - {k+1 \choose 2} \text{ for } k = 1, ..., n-1 \Big\}.
$$

Rikun states this result and verifies it using his generalized theorems that present sufficient conditions for checking certain convex envelope representations for multilinear functions. However, these results do not present the facility to derive convex envelope representations as does Theorem 2, and as demonstrated by the validation performed in Theorem 3, leading to the generalized result (13).

## 4. Concave envelope of combinatorial multilinear functions over a unit hypercube

In this section, we will use Theorem 2 to derive the concave envelope of  $\phi^m(x)$  defined in (3) over the unit hypercube H, or equivalently, we will derive the convex envelope  $\overline{\phi}_H^m(x)$  of  $\overline{\phi}^m(x) \equiv -\phi^m(x)$  over H. To apply Theorem 2, by (7b)-(7d), we need to characterize the vertices of the polyhedron defined by

$$
\Pi = \Big\{ (\pi, \pi_0) : \sum_{j \in J} \pi_j - \pi_0 \quad \forall J \subseteq N \ni |J| = k, \text{ for } k = 0, 1, \dots, m - 1,
$$

(23)

$$
\sum_{j\in J}\pi_j-\pi_0\leq -\binom{k}{m}\quad\forall J\subseteq N\ni|J|=k,\text{ for }k=m,\ldots,n.
$$

Using the consingular affine transformation

(24) 
$$
y_0 = \pi_0
$$
 and  $y_j = \pi_0 - \pi_j$   $\forall j = 1, ..., n$ ,

we will find it more convenient to equivalently characterize the vertices of the following polyhedron Y obtained by transforming Π given by (23) under (24):

(25) 
$$
Y = \left\{ (y, y_0) : \sum_{j \in J} y_j \ge (k - 1)y_0 + {k \choose m} \quad \forall J \subseteq N \ni |J| = k, \text{ for } k = 2, \dots, n, (y, y_0) \ge 0 \right\},
$$

where the nonnegativity restrictions in (25) come from (23) for  $|J| = k =$ 0 and 1 along with (24), and where throughout, we will consider that  $\frac{a}{k}$ m ``  $= 0$  whenever  $k < m$ .

Now, in order to characterize the vertices of  $Y$ , we will characterize all possible unique solutions obtainable for the linear program

(26a) **LP**: Minimize 
$$
\theta_0 y_0 + \sum_{j=1}^n \theta_j y_j
$$
,  
\n(26b) subject to  $\sum_{j \in J} y_j \ge (k-1)y_0 + \binom{k}{m} \forall J \subseteq N \ni |J| = k$ ,  
\nfor  $k = 2, ..., n$ ,  
\n(26c)  $(y, y_0) \ge 0$ .

Note that we can assume that  $\theta_j \geq 0$   $\forall j \in N$ , or else, by the nature of the constraints, LP would be unbounded if  $\theta_j < 0$  for any  $j \in N$ . Furthermore, we can assume that  $\theta_j > 0 \ \forall j \in N$  since we are interested in examining only those objective function coefficients that result in a unique (and hence a vertex) solution to LP. Hence, without loss of generality, let us characterize the optimal solution(s) to LP under the assumption that

(27) 
$$
\theta_1 \ge \theta_2 \ge \cdots \ge \theta_n > 0,
$$

and then examine all possible permutations of the type (27) in order to obtain the required vertices of  $Y$ . Toward this end, consider the following results.

**Lemma 1.** Given any  $y_0 \geq 0$ . Let LP  $(y_0)$  represent the linear program LP defined by  $(26)$  with  $y_0$  fixed at the given value, and suppose that  $(27)$ holds true. Then, an optimal extreme point solution to LP  $(y_0)$  is given by

(28) 
$$
y_1^* = 0, \ y_k^* = y_0 \text{ for } k = 2, ..., m - 1, \text{ and}
$$

$$
y_k^* = y_0 + {k - 1 \choose m - 1} \text{ for } k = m, ..., n.
$$

*Proof.* First, let us verify the feasibility of  $(28)$  to LP  $(y_0)$ . Note that (26c) holds true, and that for any  $J \subseteq N \ni |J| \equiv k \in \{2, \ldots, m-1\},\$ (26c) holds true, and that for any<br>(26b) is satisfied since we have  $\Sigma$ j∈J  $y_j^* \geq (k-1)y_0$ . Moreover, for any  $J \subseteq N \ni |J| \equiv k \in \{m, \ldots, n\}$ , we have

$$
\sum_{j \in J} y_j^* \ge (k-1)y_0 + {m-1 \choose m-1} + {m \choose m-1} + \dots + {k-1 \choose m-1}
$$
  
(29) 
$$
= (k-1)y_0 + {m \choose m} + {m \choose m-1} + {m+1 \choose m-1} + \dots + {k-1 \choose m-1}.
$$

Using the general identity that

(30) 
$$
\binom{q}{m} + \binom{q}{m-1} = \binom{q+1}{m} \text{ for any } q \geq m,
$$

and applying it inductively in (29) to pairs of the combination terms, we get that the right-hand side in (29) sums to  $(k-1)y_0 +$  $\frac{1}{k}$ m  $\frac{0}{1}$ , and so,  $y^*$ is feasible to (26b) for this case as well. Hence,  $y^*$  is feasible to LP  $(y_0)$ .

Next, let us show that  $y^*$  defined by (28) is a vertex of LP  $(y_0)$ . Toward this end consider the following n defining inequalities from  $(26)$  and let us show that  $y^*$  is a unique solution to the intersection of these n corresponding hyperplanes,

(31) 
$$
y_1 \ge 0
$$
, and  $y_1 + \sum_{j=2}^k y_j \ge (k-1)y_0 + {k \choose m}$  for  $k = 2, ..., n$ .

The first hyperplane when active yields  $y_1 = 0$  as in (28). For  $k =$  $2, \ldots, m-1$ , since the corresponding equations in (31) are  $y_1 + y_2 = y_0$ ,  $y_1 + y_2 + y_3 = 2y_0, \ldots, y_1 + y_2 + \cdots + y_{m-1} = (m-2)y_0$ , we get  $y_2 = y_3 = \cdots = y_{m-1} = y_0$ , and so again, (28) holds true. For  $k = m$ , the corresponding hyperplane in (31) gives  $y_1+y_2+\cdots+y_m = (m-1)y_0 +$  $\frac{n}{\ell}$ m , which yields from above that  $y_m = y_0 +$  $\frac{1}{m}$ m ´  $= y_0 +$  $\binom{m-1}{m}$  $m-1$ ´ as in (28).

Finally, for  $k = m + 1, \ldots, n$ , the similar difference between the hyperplane equation corresponding to k in (31) and that corresponding to  $(k-1)$ yields upon using the identity (30) for  $q \equiv k - 1$  that

$$
y_k = [(k-1)y_0 + {k \choose m}] - [(k-2)y_0 + {k-1 \choose m}]
$$
  
=  $y_0 + {k \choose m} - {k-1 \choose m} = y_0 + {k-1 \choose m-1}.$ 

Hence, the defining hyperplanes in (31) are linearly independent, yielding  $y^*$  of (28) as a unique solution, and so,  $y^*$  is a vertex of Y.

To complete the proof, it is sufficient to show that even with all but the constraints (31) of LP  $(y_0)$  relaxed,  $y^*$  is an optimal solution to this linear program. To show this, since (31) defines a polyhedral cone with its vertex at  $y^*$ , we must verify that each extreme direction  $d^t$  of this cone formed by holding all but the  $t^{th}$  inequality in (31) as active and considering the halfray feasible to the  $t^{th}$  inequality in (31) is nonimproving for  $t = 1, \ldots, n$ . Note that  $d^t = (0, \ldots, 0, 1, -1, 0, \ldots, 0)$  for  $t = 1, \ldots, n-1$ , when the two nonzeros appear in positions t and  $t + 1$ , and that  $d^n = (0, \ldots, 0, 1)$ . Hence, using (27), we see that  $\sum_{n=1}^{\infty}$  $\theta_j d_j^t = \theta_t - \theta_{t+1} \ge 0$  for  $t = 1, ..., n-1$ ,  $j=1$ and  $\sum_{n=1}^{\infty}$  $\theta_j d_j^n = \theta_n \geq 0$  for  $t = n$  as well. Hence,  $y^*$  solves LP  $(y_0)$  and this  $j=1$ completes the proof.  $\Box$ 

**Lemma 2.** Consider Problem LP defined by  $(26)$  and suppose that  $(27)$ holds true. Then, if  $y^*$  is the unique optimum to LP, we must have

(32) 
$$
y_0^* = y_1^* = \dots = y_{m-1}^* = 0
$$
, and  $y_k^* = \left(\frac{k-1}{m-1}\right)$  for  $k = m, \dots, n$ .

Proof. By Lemma 1, since (28) gives an optimal completion to a solution for LP given any  $y_0$ , we can equivalently project LP onto the space of  $y_0$ to obtain

$$
\mathbf{LP} = \underset{y_0 \ge 0}{\text{minimize}} \Big\{ \Big[ \theta_0 + \sum_{j=2}^n \theta_j \Big] y_0 + \sum_{k=m}^n {k-1 \choose m-1} \theta_k \Big\}.
$$

Hence, if  $\overline{\theta} \equiv \theta_0 +$  $\frac{n}{2}$  $j=2$  $\theta_j < 0$ , then LP is unbounded, and if  $\theta = 0$ , then LP has an infinite number of optimal solutions. Therefore, if LP has a unique optimum, we must have  $\bar{\theta} > 0$ , whence  $y_0^* = 0$ . Consequently, by Lemma 1, since (32) then gives an optimal (vertex) solution to LP, if LP has a unique optimum it must be given by  $(32)$ . This completes the proof.  $\Box$ 

We are now ready to characterize the convex envelope of  $\overline{\phi}^m(x) \equiv$  $-\phi^m(x)$  over the unit hypercube H.

**Theorem 4.** Let  $\overline{\phi}^m(x) = -\phi^m(x)$ , where  $\phi^m(x)$  is given by (3). Then

$$
\overline{\phi}_H^m(x) = \max_{k=m} \left( -\sum_{k=m}^n {k-1 \choose m-1} x_{j(k)} \right)
$$
  
for each ordered choice of indices

¡  $j(m), j(m+1), \ldots, j(n)$ ¢ selected from the set  $\{1, \ldots, n\}$ o (33)  $(j(m), j(m+1), \ldots, j(n))$  selected from the set  $\{1, \ldots, n\}$ .

Proof. By Lemma 2, and noting (27), whenever LP has a unique optimum, this optimum is of the form wherein  $y_0$  along with some  $(m-1)$  y-variables are zeros and the remaining  $(n - m + 1)$  y-variables are equal to values are zeros and the remaining<br>given collectively by  $\binom{k-1}{m-1}$  $\binom{k-1}{m-1}$  for  $k = m, \ldots, n$ . This hence characterizes the set of vertices of Y. By  $(24)$ , the set of vertices of  $\Pi$  of  $(23)$  are given by  $\pi_0 = 0$ , some  $(m - 1)$   $\pi$ -variables equal to zero, and the remaining  $\frac{1}{(k-1)}$ ່ອັ<br>`  $(n-m+1)$  π-variables equal to the values given collectively by  $$  $m-1$ for  $k = m, \ldots, n$ . Using this characterization along with Theorem 2, we obtain (33), and this completes the proof.  $\Box$ 

Remark 1. Note that the number of defining linear functions in (33) is given by

(34) 
$$
{\binom{n}{n-m+1}}(n-m+1)!
$$

**Example 2.** Consider a quadratic function  $\overline{\phi}^2(x)$  in three variables  $x_1$ ,  $x_2$ , and  $x_3$  (case of  $n = 3$ ,  $m = 2$ ). By (34),  $\overrightarrow{\phi}_H^2(x)$  has 6 defining linear functions. Each of these is given by selecting some  $(n - m + 1) = 2$ variables, and giving one of these variables a coefficient of −  $\frac{n}{1}$ 1  $=-1$ 

via  $k = m = 2$  in (33), and the other a coefficient of  $\sqrt{2}$ 1 ´  $=-2$  via  $k = n = 3$  in (33). This yields via (33) that (35)

$$
\overline{\phi}_H^2(x) = \text{maximum} \Big\{ -x_1 - 2x_2, -2x_1 - x_2, -x_1 - 2x_3, -2x_1 - x_3, -x_2 - 2x_3, -2x_2 - x_3 \Big\}.
$$

**Example 3.** Similar to Example 2, consider the case  $m = 3$ ,  $n = 4$ . By **EXAMPLE 3.** SIMMAT to E 2  $2! = 12$  terms, each term being comprised of  $(n-m+1) = 2$  variables having coefficients of  $-1$  and  $-3$  from (33). This gives

(36)

$$
\overline{\phi}_H^3(x) = \left\{ -x_1 - 3x_2, -3x_1 - x_2, -x_1 - 3x_3, -3x_1 - x_3, -x_1 - 3x_4, -3x_1 - x_4, -x_2 - 3x_3, -3x_2 - x_3, -x_2 - 3x_4, -3x_2 - x_4, -x_3 - 3x_4, -3x_3 - x_4 \right\}.
$$

## 5. Convex and concave envelopes of combinatorial multilinear functions over GUB constraints

In this section, we will extend the formulae (13) and (33) for the case where the unit hypercube  $H$  is replaced by the GUB constraints

(37) 
$$
GUB: \left\{ x : \sum_{j \in S_r} x_j \le 1 \text{ for } r = 1, ..., R, \ x \ge 0 \right\},\
$$

where  $\bigcup^R$  $i=1$  $S_i = N$ , and  $S_i \cap S_j = \emptyset \ \forall i \neq j$ , and where we are interested only in the binary solutions  $H_{GUB}$  to (37) as defined by (4). Accordingly, we assume that  $m \leq R \leq n$ , where the first inequality is assumed because otherwise, if  $R < m$ , then for each term defining  $\phi^{m}(x)$ , at least two variables must appear from some set  $S_i$ , which means that  $\phi^m(x) \equiv 0$  $\forall x \in H_{GUB}$ . Furthermore, as in (12a), let us define

(38)  
\n
$$
\phi_b^m(x) = \begin{cases}\n\phi^m(x) & \text{if } x \text{ is binary,} \\
\infty & \text{otherwise,} \n\end{cases}
$$
\nand\n
$$
\overline{\phi}_b^m(x) = \begin{cases}\n-\phi^m(x) & \text{if } x \text{ is binary,} \\
\infty & \text{otherwise,} \n\end{cases}
$$

and consider the derivation of the functions  $\phi_{bGUB}^m(x)$  and  $\overline{\phi}_{bGUB}^m(x)$  as defined in (12b). The following results provide this characterization.

**Theorem 5.** Let  $\phi_b^m(x)$  be as defined by (38), and let GUB be the set given by (37), where  $m \le R \le n$ . Then the convex envelope of  $\phi_b^m(x)$  over GUB is given by

(39)

$$
\phi_{bGuB}^{m}(x) = \text{maximum}\left\{0, \left(\frac{k}{m-1}\right) \sum_{j=1}^{n} x_j - (m-1) \binom{k+1}{m} \right\}
$$
  
for  $k = m-1, ..., R-1$ .

*Proof.* From (12b), we need to characterize vertices of  $\Pi(GUB)$ , where, from (11), we have

$$
\Pi(GUB) = \left\{ (\pi, \pi_0) : \sum_{j \in J} \pi_j - \pi_0 \le \binom{k}{m} \,\forall J \subseteq N \ni |J \cap S_i| \le 1
$$
\n
$$
\text{(40)} \quad \text{for each } i = 1, \dots, R, \text{ and } |J| = k, \text{ for } k = 0, 1, \dots, R \right\},
$$

and where as before,  $\int_{0}^{k}$ m ´  $\equiv 0$  whenever  $k < m$ . Following the proof of Theorem 3, we can construct an identical argument yielding ( $\pi = 0$ ,  $\pi_0 =$ 0) as a vertex of  $(40)$ , and that at any other vertex, the constraints in  $(40)$ corresponding to  $k = 0, 1, \ldots, m-2$  are all inactive. (Here, (17b) holds true  $\forall j \notin J_p$  where j belongs to a GUB set not represented in  $J_p$ ). Next, as in the proof of Theorem 3, suppose that for some  $k' \in \{m-1, \ldots, R-1\}$ , we have that at some vertex of  $\Pi(GUB)$ , all the constraints in (40) for  $k < k'$  are inactive, while some constraint corresponding to  $J = J_p$  with  $|J_p| = k'$  in (40) is binding.

Hence, we are given (18a) and then (18b) holds true  $\forall j \notin J_p$  where j belongs to a GUB set not represented in  $J_p$ . Using the constraints in (40) corresponding to  $k \leq k'$  along with (18), all the other constraints in (40) are then implied as in the proof of Theorem 3, and as in (20), we obtain that the possible defining hyperplanes that could determine a vertex corresponding to this case must come from the following constraints (41)  $\overline{a}$  $\mathbf{r}$ 

$$
\left\{\begin{array}{c}\text{constraints in (40) for }k = k'\\ \text{including the one for }J = J_p\end{array}\right\} \cup \left\{\begin{array}{c}\text{constraints in (18b)}\\ \text{as restarted above for}\\ \text{the present GUB situation}\end{array}\right\}.
$$

But if all the constraints in (41) are made to hold as equalities, we obtain the unique solution (22), and so, no subsystem of these equations could yield a different unique solution. Hence, as in the proof of Theorem 3, the remaining vertices of  $\Pi(GUB)$  are given by (22), but for  $k' = m 1, \ldots, R-1$ . This establishes (39) via (12b), and the proof is complete.  $\Box$ 

Theorem 6. Let  $\overline{\phi}_b^m$  $\int_{b}^{m}(x)$  be as defined by (38), and let GUB be the set given by (37), where  $m \leq R \leq n$ . Then the convex envelope of  $\overline{\phi}_{b}^{m}(x)$  over GUB is given by

$$
\overline{\phi}_{bGUB}^{m}(x) = \text{maximum} \Big\{ -\sum_{k=m}^{R} {k-1 \choose m-1} \sum_{j \in S_{i(k)}} x_j
$$
\n
$$
\text{for each ordered choice of GUB set indices}
$$
\n
$$
(42) \qquad (i(m), i(m+1), \dots, i(R)) \text{ selected from the set } \{1, \dots, R\} \Big\}.
$$

*Proof.* From (12b), we need to characterize the vertices of  $\Pi(GUB)$ , where from  $(11)$ , we have,

$$
\Pi(GUB) = \left\{ (\pi, \pi_0) : \sum_{j \in J} \pi_j - \pi_0 \le -\binom{k}{m} \,\forall J \subseteq N \ni |J \cap S_i| \le 1 \right\}
$$
\n
$$
(43) \quad \text{for each } i = 1, \dots, R, \text{ and } |J| = k, \text{ for } k = 0, 1, \dots, R \right\}.
$$

Under the transformation (24), we can equivalently seek to characterize the vertices of the set  $Y$  given below, similar to  $(25)$ .

(44)  
\n
$$
Y = \left\{ (y, y_0) : \sum_{j \in J} y_j \ge (k - 1)y_0 + {k \choose m} \,\forall J \subseteq N \ni |J \cap S_i| \le 1 \right\}
$$
\n
$$
\forall i = 1, ..., R \text{ and } |J| = k, \text{ for } k = 2, ..., R, (y, y_0) \ge 0 \right\}.
$$

Toward this end, we need to characterize all possible unique optimal solutions obtainable for the linear program of the form

(45) **LP**: minimize 
$$
\left\{\theta_0 y_0 + \sum_{j=1}^n \theta_j y_j : (y, y_0) \in Y\right\}.
$$

o

Suppose that  $y^*$  is any such optimum to (45). Let us show that for each GUB set  $S_i$ ,  $i = 1, ..., R$ , we must have that the values of  $y_j^*$  are equal to each other for all  $j \in S_i$ . To see this, fix all the variables other than  $y_j$  for  $j \in S_i$  at the values given by  $y^*$  in the linear program (45), and consider the resultant problem in these variables  $y_j, j \in S_i$ . From (44) and (45), this reduced LP is of the form

(46a) minimize 
$$
\Big\{\sum_{j\in S_i}\theta_jy_j:y_j\ge LB \quad \forall j\in S_i\Big\},\
$$

where

(46b) 
$$
LB = \underset{k=2,...,R}{\text{maximum}} \underset{\substack{J \subseteq N-S_i \\ |J| \leq 1 \ \forall j \neq i}}{\text{maximum}} \left\{ (k-1)y_0^* + {k \choose m} - \sum_{p \in J} y_p^*, 0 \right\}.
$$

Consequently, since LP is assumed to have a unique optimum  $y^*$ , by (46), we must have  $\theta_j > 0 \ \forall j \in S_i$  (and hence for all  $j \in N$ ), and moreover,  $y_j^*$ must equal LB given by (46b)  $\forall j \in S_i$ . Hence, to characterize all possible unique solutions to  $(45)$ , we can a priori set

(47) 
$$
y_0 \equiv y'_0
$$
 and  $y_j = y'_r$   $\forall j \in S_r$ , for each  $r = 1, ..., R$ 

in the LP (45), thereby reducing this to the form

$$
\mathbf{LP'} : \text{minimize } \left\{ \theta'_0 y'_0 + \sum_{r=1}^R \theta'_r y'_r : \sum_{j \in J} y'_j \ge (k-1) y'_0 + {k \choose m} \right\}
$$
  
(48) 
$$
\forall J \subseteq \{1, ..., R\} \ni |J| = k, \text{ for } k = 2, ..., R, (y', y'_0) \ge 0 \right\},
$$

where

(49) 
$$
\theta'_0 \equiv \theta_0 \text{ and } \theta'_r = \sum_{j \in S_r} \theta_j \quad \forall r = 1, ..., R.
$$

But observe that LP' of (48) is of the form of LP given in (26) for which Lemma 2 characterizes the optimum under the analogous condition (27) written for  $\theta'$ . Employing this characterization together with (47) and (24) yields a characterization of the set of vertices of  $\Pi$  as having  $\pi_0 = 0$ , some  $(m-1)$  GUB sets having their corresponding  $\pi$ -variables equal to zero, and the remaining  $(R - m + 1)$  GUB sets having the  $\pi$ -variables within each GUB set equal to each other, where these  $(R - m + 1)$  values are

 $\int k-1$ ´ given collectively by − for  $k = m, \ldots, R$ . By (12b), this establishes  $m-1$ (42), and the proof is complete.  $\Box$ 

Remark 2. Analogous to Remark 1, the number of defining linear functions in (42) is given by

(50) 
$$
\binom{R}{R-m+1}(R-m+1)!.
$$

**Example 4.** Consider a quadratic  $(m = 2)$  combinational multilinear function in  $n = 6$  variables with  $R = 3$  GUB constraint sets given by  $S_1 = \{1, 2\}, S_2 = \{3, 4\}, \text{ and } S_3 = \{5, 6\}.$  Then from (39), we directly obtain

$$
\phi_{bGUB}^2(x) = \text{maximum } \left\{0, \sum_{j=1}^6 x_j - 1, 2\sum_{j=1}^6 x_j - 3\right\},\
$$

In contrast, recall from Example 1 that  $\phi_H^2(x)$  has 3 additional defining faces in this case. Furthermore, by Theorem 6,  $\overline{\phi}_{bGUB}^2(x)$  has 6 defining linear functions (see Equation (50) of Remark 2) corresponding to the ordered GUB set index choices  $(1,2)$ ,  $(2,1)$ ,  $(1,3)$ ,  $(3,1)$ ,  $(2,3)$ , and  $(3,2)$ . By (42), these yield the characterization

$$
\overline{\phi}_{bGUB}^2(x) = \text{maximum} \left\{ - (x_1 + x_2 + 2x_3 + 2x_4), - (x_3 + x_4 + 2x_1 + 2x_2), -(x_1 + x_2 + 2x_5 + 2x_6), - (x_5 + x_6 + 2x_1 + 2x_2), -(x_3 + x_4 + 2x_5 + 2x_6), - (x_5 + x_6 + 2x_3 + 2x_4) \right\}.
$$

This is analogous to (35) of Example 2, noting (33) of Theorem 4.

#### 6. Conclusions and extensions to the general case

Thus far, we have derived explicit characterizations of convex and concave envelopes of combinatorial multilinear functions over the unit hypercube, as well as for their binary restricted versions over GUB constraints. For general multilinear functions, Theorem 2 provides a characterization for the convex envelope over a hypercube, and Corollary 1 along with (12) provides a characterization for the convex envelope of its binary restricted version over general polytopes having binary vertices. Note from these results that in general, these complete characterizations would require the enumeration of vertices of polyhedra of the type (7b) and (11b) that may not be as conveniently structured as the cases considered thus far. Indeed, as shown by Crama (1989), computing the convex envelope  $\phi_H(x)$  of a multilinear function  $\phi$  over the unit hypercube H is an NP-hard problem.

To illustrate, consider the following example of a quadratic multilinear function in  $n = 3$  variables given by

(51) 
$$
\phi(x) = x_1 x_2 - x_1 x_3 + x_2 x_3.
$$

Rikun (1996) uses this example to illustrate that the special characterizations provided by his results yield an incomplete description for this instance. Applying Theorem 3, we see that in order to completely characterize  $\phi_H(x)$ , we need to enumerate vertices of (7b), which in this instance is given by the following polyhedron, where (52a), (52b), (52c) and (52d) respectively correspond to sets  $J \subseteq N$  of cardinality 0, 1, 2, and 3.

(52a) 
$$
\Pi = \left\{ (\pi, \pi_0); -\pi_0 \leq 0, \right\}
$$

(52b) 
$$
\pi_1 - \pi_0 \leq 0, \ \pi_2 - \pi_0 \leq 0, \ \pi_3 - \pi_0 \leq 0,
$$

$$
(52c) \quad \pi_1 + \pi_2 - \pi_0 \le 1, \ \pi_1 + \pi_3 - \pi_0 \le -1, \ \pi_2 + \pi_3 - \pi_0 \le 1,
$$

$$
(52d) \quad \pi_1 + \pi_2 + \pi_3 - \pi_0 \le 1 \, \bigg\}.
$$

Enumerating the vertices of Π by systematically considering combinations of 4 linearly independent defining hyperplanes that yield a feasible solution, we obtain 7 vertices  $(\pi_1, \pi_2, \pi_3, \pi_0)$  given by  $(-1, 0, 0, 0)$ ,  $(0, 0, -1, 0)$ ,  $(1, 1, -1, 1), (-1, 1, 1, 1), (1, 2, 0, 2), (0, 2, 1, 2),$  and  $(0, 2, 0, 1)$ . This yields via (7a) that

$$
\phi_H(x) = \text{maximum} \left\{ -x_1, -x_3, x_1 + x_2 - x_3 - 1, -x_1 + x_2 + x_3 - 1, x_1 + 2x_2 - 2, 2x_2 + x_3 - 2, 2x_2 - 1 \right\}.
$$

Note that even when the coefficients  $\alpha_t$  are nonnegative  $\forall t \in T$  in (1), but do not conform to a scaled version of  $\phi^m(x)$  defined in (3), one would need to enumerate specific cases. For example, consider

$$
\phi(x) = \alpha_{12}x_1x_2 + \alpha_{13}x_1x_3 + \alpha_{23}x_2x_3,
$$

where without loss of generality, assume that the variable indices are defined so that  $0 \leq \alpha_{12} \leq \alpha_{13} \leq \alpha_{23}$ . In this case, we need to enumerate

vertices of the set  $\Pi$  given by (7b) as

$$
\Pi = \left\{ (\pi, \pi_0) : -\pi_0 \le 0, \pi_1 - \pi_0 \le 0, \pi_2 - \pi_0 \le 0, \pi_3 - \pi_0 \le 0, \pi_1 + \pi_2 - \pi_0 \le \alpha_{12}, \pi_1 + \pi_3 - \pi_0 \le \alpha_{13}, \pi_2 + \pi_3 - \pi_0 \le \alpha_{23}, \pi_1 + \pi_2 + \pi_3 - \pi_0 \le \alpha_{12} + \alpha_{13} + \alpha_{23} \right\},\
$$

and by considering various cases as before, it can be verified that this leads to the characterization (7a) given by

(54)

$$
\phi_H(x) = \text{maximum}\left\{\alpha_{12}(x_1 + x_2 + x_3) - \alpha_{12},
$$
  
\n
$$
\alpha_{13}x_1 + \alpha_{23}x_2 + (\alpha_{13} + \alpha_{23} - \alpha_{12})x_3 - (\alpha_{13} + \alpha_{23} - \alpha_{12}),
$$
  
\n
$$
\alpha_{13}x_1 + \alpha_{12}x_2 + \alpha_{13}x_3 - \alpha_{13}, \alpha_{12}x_1 + \alpha_{23}x_2 + \alpha_{23}x_3 - \alpha_{23},
$$
  
\n
$$
(\alpha_{12} + \alpha_{13})x_1 + (\alpha_{12} + \alpha_{23})x_2 + (\alpha_{13} + \alpha_{23})x_3 - (\alpha_{12} + \alpha_{13} + \alpha_{23})\right\}.
$$

While look up tables can be constructed for various special cases of this type in order to facilitate the generation of tight relaxations for general polynomial programming problems, there is another approach in which Theorem 2 could be used for constructing such relaxations. Suppose that we have a polynomial programming problem for which the (bounded) variables have been scaled to lie in the unit hypercube. Consider a particular inequality  $\phi(x) \leq \gamma$  defined by a multilinear function  $\phi$  that might relate to either the constraints or the objective function of the given polynomial program, and suppose that we decompose  $\phi(x)$  into several ( $\geq 1$ ) pieces  $\phi_p(x)$  indexed by  $p \in P$ , that are not necessarily disjoint in variables, and are such that the set  $\Pi_p$ , say, given by (7b) corresponding to  $\phi_p(x)$  is of a manageable size for each  $p \in P$ . By "manageable" we mean that either it is convenient to enumerate all the vertices of  $\Pi_p$  (perhaps by using the aforementioned look-up tables) or at least, it is convenient to generate vertices of  $\Pi_p$  via "separation problems" of the type

(55) maximize 
$$
\Big\{\sum_j \pi_{pj}\overline{x}_j - \pi_{p0} : (\pi_p, \pi_{p0}) \in \Pi_p \Big\},\
$$

where  $\bar{x}$  is a solution to some previous relaxation with respect to which a strengthened relaxation needs to be generated. Using a collection of vertices  $(\pi_p^k, \pi_{p0}^k)$  for  $k \in K_p$  of  $\Pi_p$  that are thus obtained, we can impose

(56) 
$$
\phi_p(x) \ge \text{maximum } \left\{ \sum_j \pi_{pj}^k x_j - \pi_{p0}^k \ \forall k \in K_p \right\} \ \forall p \in P.
$$

The constraints  $(56)$  can be used in combination with the original constraint  $\phi(x) \equiv$ p∈P  $\phi_p(x) \leq \gamma$  in order to generate tightened relaxations. For example in the RLT procedure of Sherali and Tuncbilek (1992), in addition to the linearized original constraint  $\phi(x) \leq \gamma$  following this scheme, the linearized form of (56) can also be similarly incorporated in order to further tighten this relaxation. Such considerations need further investigation, and will be explored in future research.

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